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Critically evaluated theoretical atomic properties of Y III

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A systematic study of Y III atomic properties is carried out using high-precision relativistic all-order method. Recommended values and estimates of their uncertainties are provided for a large number of electric-dipole reduced matrix elements, transition rates, and oscillator strengths for allowed transitions between ns, np_j, nd_j, nf_j, and ng_j levels with $n \leq 8$. The lifetimes of these levels are also evaluated. Electric-quadrupole and magnetic-dipole matrix elements are calculated to determine lifetimes of the $4d_{5/2}$ and $5s$ metastable levels. The ground state E1, E2, and E3 static polarizabilities are calculated. This work provide recommended values critically evaluated for their accuracy for a number of Y III atomic properties for use in theoretical modeling as well as planning and analysis of various experiments. We hope that the present study will stimulate further exploration of Y III for various applications owing to its interesting structure of different low-lying metastable levels.

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I. INTRODUCTION

We report results of *ab initio* calculations of excitation energies, transition rates, lifetimes, and multipole polarizabilities in Rb-like yttrium. Rb and Rb-like ions are excellent systems for tests of high-precision theories and benchmark comparisons with experiments owing to relatively simple electronic structure. Critically evaluated theoretical lifetimes, hyperfine constants, multipole polarizabilities, and blackbody radiation shift in the ^{87}Rb frequency standard in neutral rubidium were reported in Refs. [1, 2]. Accurate values of Rb atomic properties are of significant present interest owing to the importance of this system for ultracold atom studies [4–7]. In 2010, a systematic study of Rb-like Sr^+ atomic properties was carried out [3] using high-precision relativistic all-order method where all single, double, and partial triple excitations of the Dirac-Fock wave functions are included to all orders of perturbation theory. The properties of Sr^+ are of present interest of many applications in various fields such as optical frequency standards, quantum information, and astronomy.

Both Rb and Rb-like Sr^+ have [Kr]$4s$ ground state, where [Kr]=$1s^22s^22p^63s^23p^63d^{10}4s^24p^6$. We omit [Kr] from the electronic configurations below. The first excited configuration of Rb is $5p$, while the first excited configuration of Sr^+ is $4d$. Availability of low-lying metastable $4d$ levels in Sr^+ led to numerous applications mentioned above. The level scheme of Rb-like Y III is different from both Rb and Rb-like Sr^+: the ground state is $4d_{3/2}$, and the first two excited states are $4d_{5/2}$ and $5s$. The next configuration is $5p$. Therefore, two different low-lying metastable states are available. The $4d$ fine-structure splitting is large, 724 cm^{-1} and the lifetime of $4d_{5/2}$ level is very long, 244 seconds. The $5s$ level is also metastable, with 11 s lifetime. It would be interesting to explore the possibility of using $4d_{3/2}$ - $4d_{5/2}$ states for quantum memory owing to a very long lifetime of the $4d_{5/2}$ level. Metastable levels of ions are also of interest to astrophysics and plasma diagnostics.

We start with a brief review of previous studies. Recently, lifetime measurements and calculations of Y III ion properties were presented by Biémont *et al.* [9]. The theoretical results were in good agreement with new laser measurements of two $5p$ levels obtained in this work and with previous beam-foil results for $5d$ and $6s$ levels. Theoretical calculations of the lowest metastable state lifetimes in Y III were reported by Sahoo *et al.* [12]. Lifetimes of the $4d_{5/2}$ and $5s$ levels were determined using the relativistic coupled-cluster theory [12]. The Weakest Bound Electron Potential Model (WBEPM) theory was used in Ref. [10] to calculate transition probabilities and oscillator strengths for a number of Y III transitions. Theoretical determination of oscillator strengths for the principal series of rubidium-like ions by the Dirac-Fock method was reported by Zilitis [13].

The Rb-like Y III has been studied in a number of earlier experimental and theoretical [11, 14–21] papers. Dipole transition probabilities and oscillator strengths along the rubidium isoelectronic sequence were evaluated by Lindgård and Nielsen [15]. To make the required predictions for atoms and ions of alkali sequences authors found that the Coulomb approximation, originally applied by Bates and Damgaard [22], offers a sensible compromise between accuracy and computational effort. Relativistic single-configuration Hartree-Fock oscillator strengths for the lowest $ns - np_j$ transitions in the first few members of the rubidium ($n = 5$) isoelec-

tronic sequences had been studied by Migdalek and Bailis [16]. The effect of core polarization of the atom or ion by the valence electron was included by introducing a polarization potential in the one-electron Hamiltonian and by employing the corresponding correction for the dipole moment operator in the transition matrix elements. Quasi-relativistic local spin density functional with correlation energy was used by Sen and Puri [17] to calculate the $ns - np_j$ dipole oscillator strength in the Rb isoelectronic series. Oscillator strengths for selected transitions of Y III were determined by Brage *et al.* [19] using the multiconfiguration Hartree-Fock techniques. The importance of including an accurate treatment of the core-valence correlation was emphasized by authors. The oscillator strengths of the resonance transitions were calculated by Zilitis [21] using the Dirac-Fock method for the first ten terms of the rubidium isoelectronic sequence. Lifetime measurements, using beam-foil excitation, were reported by Maniak *et al.* [11] for doubly charged yttrium, Y III.

None of the previous studies listed above, except recent lifetime calculations of [12], were carried out by high-precision *ab initio* methods.

In the present work, relativistic high-precision all-order (linearized coupled-cluster) method is used to calculate atomic properties of doubly ionized yttrium for the ns, np_j, nd_j, nf_j, and ng_j states with $n \leq 9$. Excitation energies and lifetimes are calculated for the first 46 excited states. The reduced electric-dipole matrix elements, line strengths, oscillator strengths, and transition rates are determined for allowed transitions between these levels. The M1 $4d_{3/2} - 4d_{5/2}$, $4d_{3/2} - 5s$ and E2 $4d_{3/2} - 4d_{5/2}$, $4d_j - 5s$ matrix elements are evaluated and used to calculate lifetimes of the metastable $4d_{5/2}$ and $5s$ levels. The E1, E2, and E3 static polarizabilities are determined for the $5s$ level. Scalar and tensor polarizabilities of the $4d_j$ states of Rb-like Y III are evaluated. The uncertainties of the final values are estimated for all properties.

The main motivation for this work is to provide recommended values critically evaluated for their accuracy for a number of atomic properties via a systematic high-precision study for use in theoretical modeling as well as planning and analysis of various experiments that may utilize interesting structure of Y III levels.

II. THIRD-ORDER AND ALL-ORDER CALCULATIONS OF ENERGIES

Energies of nl_j states in Y III are evaluated for $n \leq 8$ and $l \leq 4$ using both third-order relativistic many-body perturbation theory (RMBPT) and the single-double (SD) all-order method discussed in Refs. [1–3]. The B-splines [23] are used to generate a complete set of Dirak-Fock (DF) basis orbitals for use in the evaluation of all atomic properties. The present calculation of the transition rates and lifetimes required accurate representation of rather highly-excited states, such as $8lj$, leading to the use of the large R = 110 a.u. cavity for the generation of the finite basis set and higher number ($N = 70$) of splines to produce high-accuracy single-particle orbitals. Results of our energy calculations are summarized in Table I. The third-order values $E^{(3)}_{\rm tot}$ include the lower-order DF energies $E^{(0)}$, second-order and third-order Coulomb correlation energies $E^{(2)}$ and $E^{(3)}$, first-order and second-order Breit corrections $B^{(1)}$ and $B^{(2)}$, and an estimated Lamb shift contribution, $E^{(\rm LS)}$. The Lamb shift $E^{(\rm LS)}$ is calculated as the sum of the one-electron self-energy and the first-order vacuum-polarization energy. The self-energy contribution is estimated for the ns and np orbitals by interpolating among the values obtained by Mohr [25, 26, 27] using Coulomb wave functions. For this purpose, an effective nuclear charge $Z_{\rm eff}$ is obtained by finding the value of $Z_{\rm eff}$ required to give a Coulomb orbital with the same average $\langle r \rangle$ as the DF orbital. The vacuum-polarization contribution is calculated from the Uehling potential using the results of Fullerton and Rinker [24]. It should be noted that the values of $E^{(\rm LS)}$ are very small, 12 cm^{-1} for the $5s$ state and 2 cm^{-1} for the $6s$ state. They are negligible for all other levels. The sum of the seven terms $E^{(0)}$, $E^{\rm SD}$, $E^{(3)}_{\rm extra}$, $B^{(1)}$, $B^{(2)}$, and $E^{(\rm LS)}$ is our final all-order result $E^{\rm SD}_{\rm tot}$, listed in the third column of Table I. Recommended energies from the National Institute of Standards and Technology (NIST) database [28] are given in the column labeled $E_{\rm NIST}$. Differences between our third-order and all-order calculations and experimental data, $\delta E^{(3)} = E^{(3)}_{\rm tot} - E_{\rm NIST}$ and $\delta E^{\rm SD} = E^{\rm SD}_{\rm tot} - E_{\rm NIST}$, are given in the two final columns of Table I, respectively.

We calculate $E^{(2)}$ with higher numerical accuracy since the largest correlation contribution to the valence energy comes from the second-order term. The second-order energy includes partial waves up to $l_{\rm max} = 8$ and is extrapolated to account for contributions from higher partial waves (see, for example, Refs. [29, 30] for details of the extrapolation procedure). As an example of the convergence of $E^{(2)}$ with the number of partial waves l, consider the $4d_{3/2}$ state. Calculations of $E^{(2)}$ with $l_{\rm max} = 6$ and 8 yield $E^{(2)}(4d_{3/2})$ = -10903.8 and -11101.4 cm^{-1}, respectively. Extrapolation of these calculations yields -11179.1 and -11170.1 cm^{-1}, respectively. Thus, in this particular case, we have a numerical uncertainty in $E^{(2)}(4d_{3/2})$ of 8.5 cm^{-1}. The same value of numerical uncertainty is found for $E^{(2)}(4d_{5/2})$. It should be noted that this is the largest uncertainty among all states considered in Table I; smaller (0.8 cm^{-1}, 0.3 cm^{-1}, and 1.1 cm^{-1}) uncertainties are obtained for the $5s$, $5p$, and $5d$ states and much smaller uncertainties (0.2 cm^{-1}, 0.1 cm^{-1}, and 0.4 cm^{-1}) are obtained for the $6s$, $6p$, and $6d$ states owing to much smaller contributions of higher partial waves. Owing to numerical complexity, we restrict $l \leq l_{\rm max} = 6$ in the third-order and all-order calculations. As noted above, the second-order contribution dominates $E^{\rm SD}$; therefore, we can use the extrapolated value of the $E^{(2)}$ described above to account for the contributions of the higher par-

TABLE I: The total removal energies of Rb-like Y III ($E^{(3)}_{\rm tot} = E^{(0)} + E^{(2)} + E^{(3)} + B^{(1)} + B^{(2)} + E^{(\rm LS)}$, $E^{\rm SD}_{\rm tot} = E^{(0)} + E^{\rm SD} + E^{(3)}_{\rm extra} + B^{(1)} + B^{(2)} + E^{(\rm LS)}$) are compared with recommended NIST energies $E_{\rm NIST}$ [8], $\delta E = E_{\rm tot}$ - $E_{\rm NIST}$. Units: cm^{-1}.

nlj	$E^{(3)}_{\rm tot}$	$E^{\rm SD}_{\rm tot}$	$E_{\rm NIST}$	$\delta E^{(3)}$	$\delta E^{\rm SD}$
$4d_{3/2}$	-165039	-165336	-165540	502	204
$4d_{5/2}$	-164329	-164625	-164816	487	192
$4f_{5/2}$	-64143	-64410	-64449	306	39
$4f_{7/2}$	-64151	-64414	-64452	301	39
$5s_{1/2}$	-157513	-157852	-158073	560	221
$5p_{1/2}$	-123712	-124016	-124139	427	123
$5p_{3/2}$	-122178	-122469	-122586	408	117
$5d_{3/2}$	-76999	-77084	-77161	162	77
$5d_{5/2}$	-76801	-76887	-76962	161	75
$5f_{5/2}$	-41137	-41323	-41348	211	25
$5f_{7/2}$	-41141	-41323	-41347	206	24
$5g_{7/2}$	-39690	-39698	-39704	14	6
$5g_{9/2}$	-39690	-39698	-39704	14	6
$6s_{1/2}$	-78673	-78729	-78823	150	94
$6p_{1/2}$	-66221	-66217	-66195	-27	-22
$6p_{3/2}$	-65454	-65533	-65597	143	64
$6d_{3/2}$	-46526	-46566	-46604	78	38
$6d_{5/2}$	-46434	-46474	-46511	77	37
$6f_{5/2}$	-28505	-28629	-28646	141	17
$6f_{7/2}$	-28507	-28629	-28645	137	16
$6g_{7/2}$	-27558	-27564	-27567	9	3
$6g_{9/2}$	-27558	-27564	-27567	9	3
$7s_{1/2}$	-47563	-47580	-47625	63	46
$7p_{1/2}$	-41427	-41462	-41499	72	36
$7p_{3/2}$	-41133	-41166	-41202	69	36
$7d_{3/2}$	-31290	-31313	-31334	44	21
$7d_{5/2}$	-31239	-31262	-31283	43	21
$7f_{5/2}$	-20878	-20963	-20975	97	12
$7f_{7/2}$	-20879	-20962	-20973	94	11
$7g_{7/2}$	-20241	-20244	-20246	5	2
$7g_{9/2}$	-20241	-20244	-20246	5	1
$8s_{1/2}$	-31910	-31913	-31941	32	29
$8p_{1/2}$	-28465	-28484	-28504	39	20
$8p_{3/2}$	-28297	-28315	-28335	38	20
$8d_{3/2}$	-22510	-22524	-22536	26	12
$8d_{5/2}$	-22479	-22493	-22505	26	12
$8f_{5/2}$	-15936	-15996	-16004	68	8
$8f_{7/2}$	-15937	-15995	-16003	66	7
$8g_{7/2}$	-15492	-15494	-15495	3	1
$8g_{9/2}$	-15492	-15494	-15495	3	1
$9s_{1/2}$	-22903	-22905	-22920	17	15
$9p_{1/2}$	-20777	-20787	-20799	23	13
$9p_{3/2}$	-20671	-20678	-20693	22	15
$9d_{3/2}$	-16977	-16986			
$9d_{5/2}$	-16957	-16966			
$10s_{1/2}$	-17241	-17241			

tial waves. We note that the contributions of higher partial waves to removal energies are very large for the $4d_{3/2}$ and $4d_{5/2}$ states: $l > 6$ contribution is 266 cm^{-1} and 263 cm^{-1}, respectively. Therefore, they must be included in a high-precision calculations. Restricting basis sets in coupled-cluster calculations to only a few first partial waves will lead to a significant loss of numerical accuracy.

The column labeled $\delta E^{\rm SD}$ in Table I gives differences between our *ab initio* results and the available experimental values [28]. The all-order values for removal energies are in excellent agreement with experimental data. The ionization potential agrees with experiment to 0.12%. The SD results agree better with NIST values than do the third-order MBPT results (the ratio of $\delta E^{(3)}/\delta E^{\rm SD}$ is about 2-3 for some of cases), illustrating the importance of fourth and higher-order correlation corrections.

III. ELECTRIC-DIPOLE MATRIX ELEMENTS, OSCILLATOR STRENGTHS, TRANSITION RATES, AND LIFETIMES IN RB-LIKE Y III

A. Electric-dipole matrix elements

In Table II, we list our recommended values for 138 E1 $ns - n'p$, $nd - n'p$, $nd - n'f$, and $ng - n'f$ transitions. The absolute values in atomic units ($a_0 e$) are given in all cases. We note that we have calculated about 260 E1 matrix elements to consider all dipole transitions between the ns, np_j, nd_j, nf_j, and ng_j states with $n \leq 8$. We refer to these values as recommended matrix elements. We only list the matrix elements that give significant contributions to the atomic lifetimes and polarizabilities calculated in the other sections. To evaluate the uncertainties of these values, we carried out a number of calculations using different methods of increasing accuracy: lowest-order DF, second-order relativistic many-body perturbation theory (RMBPT), third-order RMBPT, and all-order methods. The MBPT calculations are carried out using the method described in Ref. [31]. Comparisons of the values obtained in different approximations allow us to evaluated the size of the second, third, and higher-order correlation corrections, as well as estimate the uncertainties in the final values.

The evaluation of the uncertainty of the matrix elements in this approach was described in detail in [2, 32]. It is based on four different all-order calculations that included two *ab initio* all-order calculations with and without the inclusion of the partial triple excitations and two calculations that included semiempirical estimate of high-order correlation corrections starting from both *ab initio* runs. The differences of these four values for each transition were used to estimate uncertainty in the final results based on the algorithm that accounted for importance of the specific dominant contributions.

The column labelled "%" of Table II gives relative uncertainties of the final values $Z^{\rm final}$ in per cent. The values of uncertainties for the 138 E1 138 E1 $ns - n'p$, $nd - n'p$, $nd - n'f$, and $ng - n'f$ transitions given in Table II are smaller than 1%. We find that the uncertainties are 0.1-0.3% for the $ns - n'p$ and $ng - n'f$ transitions. Larger uncertainties (0.5% - 0.7%) occur for some of the the $nd - n'p$ and $nd - n'f$transitions owing to the increased relative size of the correlation corrections. The

TABLE II: Recommended values of the reduced electric-dipole matrix elements in Rb-like Y III in atomic units. Final recommended values and their uncertainties are given in the $Z^{\rm final}$ column. The DF values are displayed in the $Z^{\rm DF}$ column. The column (%) gives relative uncertainties of the final values in %. Absolute values are given.

Transition	DF	Final	%	Transition	DF	Final	%	Transition	DF	Final	%
$6s_{1/2}-5p_{1/2}$	1.7038	1.684(7)	0.41	$7d_{3/2}-9p_{3/2}$	0.3497	0.370(3)	0.80	$7d_{5/2}-4f_{7/2}$	0.8837	0.858(5)	0.56
$6s_{1/2}-5p_{3/2}$	2.5296	2.502(7)	0.30	$7d_{5/2}-6p_{3/2}$	2.2414	2.124(8)	0.37	$7d_{5/2}-5f_{5/2}$	1.5748	1.454(6)	0.43
$6s_{1/2}-6p_{1/2}$	5.3430	5.13(1)	0.21	$7d_{5/2}-7p_{3/2}$	13.5982	13.47(4)	0.31	$7d_{5/2}-5f_{7/2}$	7.0310	6.50(2)	0.37
$6s_{1/2}-6p_{3/2}$	7.5186	7.23(2)	0.22	$7d_{5/2}-8p_{3/2}$	20.6724	20.18(4)	0.19	$7d_{5/2}-6f_{5/2}$	6.2783	6.129(8)	0.14
$7s_{1/2}-5p_{1/2}$	0.4896	0.4967(7)	0.15	$8d_{3/2}-6p_{1/2}$	0.8518	0.793(5)	0.68	$7d_{5/2}-6f_{7/2}$	28.0759	27.41(4)	0.13
$7s_{1/2}-5p_{3/2}$	0.7089	0.717(1)	0.16	$8d_{3/2}-6p_{3/2}$	0.3709	0.344(2)	0.67	$7d_{5/2}-8f_{7/2}$	2.7571	3.08(2)	0.71
$7s_{1/2}-6p_{1/2}$	3.3308	3.277(7)	0.20	$8d_{3/2}-7p_{1/2}$	2.5082	2.438(6)	0.24	$8d_{3/2}-4f_{5/2}$	0.3707	0.364(2)	0.54
$7s_{1/2}-6p_{3/2}$	4.9179	4.843(6)	0.13	$8d_{3/2}-7p_{3/2}$	1.1117	1.078(3)	0.25	$8d_{3/2}-5f_{5/2}$	1.5003	1.423(7)	0.50
$7s_{1/2}-7p_{1/2}$	8.5194	8.338(9)	0.11	$8d_{3/2}-8p_{3/2}$	6.2907	6.27(2)	0.28	$8d_{3/2}-6f_{5/2}$	9.4187	8.59(6)	0.66
$7s_{1/2}-7p_{3/2}$	11.9645	11.71(1)	0.13	$8d_{3/2}-9p_{1/2}$	22.0289	21.59(4)	0.16	$8d_{3/2}-7f_{5/2}$	33.0243	32.48(3)	0.08
$8s_{1/2}-6p_{1/2}$	0.8822	0.880(2)	0.17	$8d_{3/2}-9p_{3/2}$	9.7254	9.52(2)	0.16	$8d_{5/2}-4f_{5/2}$	0.0986	0.0969(6)	0.59
$8s_{1/2}-6p_{3/2}$	1.2660	1.262(2)	0.13	$8d_{5/2}-6p_{3/2}$	1.1237	1.042(7)	0.70	$8d_{5/2}-4f_{7/2}$	0.4405	0.433(3)	0.64
$8s_{1/2}-7p_{1/2}$	5.4059	5.312(4)	0.07	$8d_{5/2}-7p_{3/2}$	3.3497	3.251(8)	0.25	$8d_{5/2}-5f_{5/2}$	0.3986	0.378(2)	0.48
$8s_{1/2}-7p_{3/2}$	7.9596	7.833(8)	0.10	$8d_{5/2}-8p_{3/2}$	18.7416	18.69(6)	0.31	$8d_{5/2}-5f_{7/2}$	1.7806	1.690(8)	0.45
$8s_{1/2}-8p_{1/2}$	12.4092	12.227(6)	0.05	$8d_{5/2}-9p_{3/2}$	29.3222	28.72(5)	0.17	$8d_{5/2}-6f_{5/2}$	2.4868	2.27(1)	0.63
$8s_{1/2}-8p_{3/2}$	17.4052	17.147(7)	0.04					$8d_{5/2}-6f_{7/2}$	11.1025	10.14(6)	0.56
$9s_{1/2}-6p_{1/2}$	0.4669	0.4694(8)	0.17	$5d_{3/2}-4f_{5/2}$	8.5163	7.99(2)	0.27	$8d_{5/2}-7f_{5/2}$	8.8405	8.692(8)	0.09
$9s_{1/2}-6p_{3/2}$	0.6659	0.668(1)	0.18	$5d_{3/2}-5f_{5/2}$	2.6722	2.85(2)	0.55	$8d_{5/2}-7f_{7/2}$	39.5365	38.87(3)	0.09
$9s_{1/2}-7p_{1/2}$	1.3707	1.359(2)	0.13	$5d_{3/2}-6f_{5/2}$	1.5933	1.649(6)	0.35				
$9s_{1/2}-7p_{3/2}$	1.9581	1.941(3)	0.13	$5d_{3/2}-7f_{5/2}$	1.0835	1.099(7)	0.63	$5g_{7/2}-4f_{5/2}$	10.4469	9.67(4)	0.39
$9s_{1/2}-8p_{1/2}$	7.9371	7.806(5)	0.07	$5d_{3/2}-8f_{5/2}$	0.8041	0.807(4)	0.53	$5g_{7/2}-4f_{7/2}$	2.0094	1.861(7)	0.36
$9s_{1/2}-8p_{3/2}$	11.6674	11.49(1)	0.09	$5d_{5/2}-4f_{5/2}$	2.2776	2.138(6)	0.28	$5g_{7/2}-5f_{5/2}$	14.1754	14.34(2)	0.12
$9s_{1/2}-9p_{1/2}$	17.0142	16.823(7)	0.04	$5d_{5/2}-4f_{7/2}$	10.1829	9.56(3)	0.27	$5g_{7/2}-5f_{7/2}$	2.7287	2.761(3)	0.12
$9s_{1/2}-9p_{3/2}$	23.8433	23.57(1)	0.04	$5d_{5/2}-5f_{5/2}$	0.7290	0.775(4)	0.47	$5g_{9/2}-4f_{7/2}$	11.8882	11.01(4)	0.35
				$5d_{5/2}-5f_{7/2}$	3.2670	3.47(1)	0.42	$5g_{9/2}-5f_{7/2}$	16.1428	16.33(2)	0.12
$4d_{3/2}-5p_{1/2}$	2.2476	1.945(7)	0.36	$5d_{5/2}-6f_{5/2}$	0.4315	0.446(1)	0.30	$6g_{7/2}-5f_{7/2}$	2.4300	2.16(2)	0.78
$4d_{3/2}-5p_{3/2}$	0.9889	0.857(3)	0.36	$5d_{5/2}-6f_{7/2}$	1.9322	1.993(5)	0.26	$6g_{7/2}-6f_{5/2}$	25.3143	25.51(2)	0.09
$4d_{5/2}-5p_{3/2}$	2.9988	2.61(1)	0.39	$5d_{5/2}-7f_{5/2}$	0.2926	0.296(2)	0.65	$6g_{7/2}-6f_{7/2}$	4.8726	4.910(4)	0.08
$5d_{3/2}-6p_{1/2}$	5.6762	5.43(1)	0.25	$5d_{5/2}-7f_{7/2}$	1.3099	1.325(9)	0.65	$6g_{9/2}-6f_{7/2}$	28.8263	29.05(2)	0.08
$5d_{3/2}-6p_{3/2}$	2.5014	2.394(6)	0.24	$5d_{5/2}-8f_{5/2}$	0.2168	0.217(1)	0.54	$7g_{7/2}-4f_{5/2}$	1.7519	1.749(6)	0.32
$5d_{3/2}-7p_{3/2}$	0.2025	0.198(1)	0.74	$5d_{5/2}-8f_{7/2}$	0.9705	0.971(5)	0.54	$7g_{7/2}-4f_{7/2}$	0.3373	0.337(1)	0.35
$5d_{5/2}-6p_{3/2}$	7.5581	7.24(2)	0.26	$6d_{3/2}-4f_{5/2}$	3.1208	2.958(7)	0.24	$7g_{7/2}-5f_{5/2}$	4.7592	4.55(2)	0.33
$5d_{5/2}-7p_{3/2}$	0.5916	0.578(4)	0.77	$6d_{3/2}-5f_{5/2}$	15.3140	14.77(3)	0.18	$7g_{7/2}-5f_{7/2}$	0.9157	0.876(3)	0.32
$6d_{3/2}-6p_{1/2}$	6.7192	6.58(3)	0.41	$6d_{3/2}-7f_{5/2}$	1.9122	2.08(1)	0.66	$7g_{7/2}-7f_{5/2}$	37.8469	38.01(2)	0.06
$6d_{3/2}-6p_{3/2}$	3.0914	3.03(1)	0.33	$6d_{3/2}-8f_{5/2}$	1.3145	1.407(7)	0.49	$7g_{7/2}-7f_{7/2}$	7.2846	7.316(4)	0.05
$6d_{3/2}-7p_{1/2}$	10.0845	9.79(2)	0.21	$6d_{5/2}-4f_{5/2}$	0.8241	0.781(2)	0.20	$7g_{9/2}-4f_{7/2}$	1.9958	1.992(7)	0.35
$6d_{3/2}-7p_{3/2}$	4.4482	4.317(8)	0.19	$6d_{5/2}-4f_{7/2}$	3.6802	3.494(7)	0.19	$7g_{9/2}-5f_{7/2}$	5.4175	5.18(2)	0.32
$6d_{3/2}-8p_{3/2}$	0.2728	0.281(2)	0.66	$6d_{5/2}-5f_{5/2}$	4.0978	3.953(8)	0.19	$7g_{9/2}-7f_{7/2}$	43.0958	43.28(2)	0.05
$6d_{5/2}-6p_{3/2}$	9.2223	9.04(3)	0.36	$6d_{5/2}-5f_{7/2}$	18.3233	17.68(3)	0.18	$8g_{7/2}-4f_{5/2}$	1.1397	1.147(6)	0.52
$6d_{5/2}-7p_{3/2}$	13.4250	13.03(3)	0.21	$6d_{5/2}-7f_{5/2}$	0.5199	0.565(3)	0.59	$8g_{7/2}-4f_{7/2}$	0.2195	0.221(1)	0.45
$6d_{5/2}-8p_{3/2}$	0.7860	0.812(6)	0.74	$6d_{5/2}-7f_{7/2}$	2.3300	2.52(1)	0.51	$8g_{7/2}-6f_{5/2}$	6.0542	5.61(4)	0.70
$7d_{3/2}-6p_{1/2}$	1.6821	1.598(6)	0.35	$6d_{5/2}-8f_{5/2}$	0.3562	0.380(2)	0.43	$8g_{7/2}-6f_{7/2}$	1.1645	1.079(7)	0.67
$7d_{3/2}-6p_{3/2}$	0.7428	0.703(3)	0.36	$6d_{5/2}-8f_{7/2}$	1.5956	1.700(6)	0.36	$8g_{7/2}-8f_{5/2}$	52.0486	52.13(2)	0.04
$7d_{3/2}-7p_{1/2}$	9.8984	9.82(4)	0.37	$7d_{3/2}-4f_{5/2}$	0.7445	0.722(3)	0.48	$8g_{7/2}-8f_{7/2}$	10.0177	10.033(4)	0.04
$7d_{3/2}-7p_{3/2}$	4.5619	4.52(1)	0.28	$7d_{3/2}-5f_{5/2}$	5.9643	5.51(3)	0.46	$8g_{9/2}-4f_{7/2}$	1.2986	1.306(6)	0.46
$7d_{3/2}-8p_{1/2}$	15.5299	15.17(3)	0.19	$7d_{3/2}-6f_{5/2}$	23.4567	22.90(3)	0.13	$8g_{9/2}-6f_{7/2}$	6.8892	6.38(4)	0.67
$7d_{3/2}-8p_{3/2}$	6.8538	6.69(1)	0.17	$7d_{5/2}-4f_{5/2}$	0.1978	0.192(1)	0.52	$8g_{9/2}-8f_{7/2}$	59.2653	59.36(2)	0.04

values of uncertainties in Rb-like Y III are slightly smaller than the values of uncertainties in Rb-like Sr II [3] and neutral Rb [2]. Our final results and their uncertainties are used to calculate the recommended values of the transition rates, oscillator strengths, and lifetimes discussed below.

B. Transition rates and oscillator strengths

We combine recommended NIST energies [8] and our final values of the matrix elements listed in Table II to calculate weighted transition rates gA_r and weighted oscillator strengths gf. The weighted transition rates gA_r

TABLE III: Weighted transition rates gA_r (s^{-1}) in Rb-like Y III calculated using our recommended values of reduced electric-dipole matrix elements. The relative uncertainties of the final values are listed in column "Unc." in %. Lowest-order DF values are listed in column "DF". The vacuum wavelengths λ in Å from NIST compilation [8] are listed for reference. Numbers in brackets represent powers of 10.

Transition		λ	gA_r	Unc.	Transition		λ	gA_r	Unc.	Transition		λ	gA_r	Unc.
Lower	Upper	Å	s^{-1}	%	Lower	Upper	Å	s^{-1}	%	Lower	Upper	Å	s^{-1}	%
$5p_{1/2}$	$9s_{1/2}$	987.95	7.18[7]	0.2	$5p_{1/2}$	$6s_{1/2}$	2206.72	5.35[8]	0.8	$4d_{5/2}$	$5f_{5/2}$	809.92	3.67[8]	0.9
$5p_{3/2}$	$9s_{1/2}$	1003.35	1.40[8]	0.3	$6p_{3/2}$	$8d_{3/2}$	2322.31	1.91[7]	1.3	$4d_{5/2}$	$5f_{7/2}$	809.92	7.38[9]	0.9
$5p_{3/2}$	$8s_{1/2}$	1103.21	2.33[8]	0.3	$4f_{7/2}$	$8d_{5/2}$	2383.95	2.81[7]	1.3	$5p_{1/2}$	$8d_{3/2}$	984.23	1.33[8]	1.3
$5p_{1/2}$	$7s_{1/2}$	1306.95	2.24[8]	0.3	$4f_{5/2}$	$8d_{3/2}$	2385.91	1.98[7]	1.1	$4d_{3/2}$	$4f_{5/2}$	989.20	1.06[10]	0.4
$5p_{3/2}$	$7s_{1/2}$	1334.04	4.38[8]	0.3	$5d_{3/2}$	$5f_{5/2}$	2792.26	7.55[8]	1.1	$4d_{5/2}$	$4f_{5/2}$	996.34	7.60[8]	0.4
$5d_{3/2}$	$8f_{5/2}$	1635.14	3.02[8]	1.1	$5d_{3/2}$	$7p_{1/2}$	2804.09	1.40[7]	2.0	$4d_{5/2}$	$4f_{7/2}$	996.37	1.52[10]	0.5
$5d_{5/2}$	$8f_{7/2}$	1640.43	4.33[8]	1.1	$5d_{5/2}$	$5f_{5/2}$	2807.83	5.50[7]	0.9	$5p_{1/2}$	$7d_{3/2}$	1077.52	2.66[8]	1.1
$5d_{3/2}$	$7f_{5/2}$	1779.80	4.34[8]	1.3	$5d_{5/2}$	$5f_{7/2}$	2807.83	1.10[9]	0.8	$5p_{1/2}$	$6d_{3/2}$	1289.73	6.83[8]	0.9
$5d_{5/2}$	$7f_{7/2}$	1786.06	6.25[8]	1.3	$4f_{7/2}$	$7d_{5/2}$	3014.82	5.45[7]	1.1	$5p_{3/2}$	$6d_{5/2}$	1314.50	1.13[9]	0.9
$5d_{5/2}$	$7f_{5/2}$	1786.11	3.12[7]	1.3	$4f_{5/2}$	$7d_{3/2}$	3019.74	3.84[7]	1.0	$5d_{5/2}$	$8p_{3/2}$	2056.46	1.71[7]	2.2
$5d_{3/2}$	$6f_{5/2}$	2061.24	6.29[8]	0.7	$6d_{3/2}$	$8f_{5/2}$	3268.04	1.15[8]	1.0	$5p_{1/2}$	$5d_{3/2}$	2128.65	3.09[9]	0.6
$5d_{5/2}$	$6f_{7/2}$	2069.64	9.08[8]	0.5	$6d_{5/2}$	$8f_{7/2}$	3277.76	1.66[8]	0.7	$5p_{3/2}$	$5d_{5/2}$	2191.86	5.32[9]	0.6
$5d_{5/2}$	$6f_{5/2}$	2069.72	4.54[7]	0.6	$6d_{5/2}$	$8f_{5/2}$	3277.94	8.32[6]	0.9	$5p_{3/2}$	$5d_{3/2}$	2201.44	5.89[8]	0.5
$4f_{7/2}$	$7g_{7/2}$	2262.11	1.98[7]	0.7	$6d_{3/2}$	$7f_{5/2}$	3901.85	1.48[8]	1.3	$6p_{3/2}$	$8d_{5/2}$	2320.63	1.76[8]	1.4
$4f_{7/2}$	$7g_{9/2}$	2262.11	6.94[8]	0.7	$6d_{5/2}$	$7f_{7/2}$	3915.69	2.15[8]	1.0	$6p_{1/2}$	$8d_{3/2}$	2290.50	1.06[8]	1.4
$4f_{5/2}$	$7g_{7/2}$	2262.28	5.36[8]	0.6	$6d_{5/2}$	$7f_{5/2}$	3915.96	1.08[7]	1.2	$4d_{3/2}$	$5p_{3/2}$	2328.02	1.18[8]	0.7
$5p_{3/2}$	$6s_{1/2}$	2285.05	1.06[9]	0.6	$4f_{7/2}$	$5g_{7/2}$	4040.73	1.06[8]	0.7	$4d_{5/2}$	$5p_{3/2}$	2367.94	1.04[9]	0.8
$6p_{1/2}$	$9s_{1/2}$	2310.80	3.62[7]	0.3	$4f_{7/2}$	$5g_{9/2}$	4040.74	3.72[9]	0.7	$4d_{3/2}$	$5p_{1/2}$	2415.37	5.44[8]	0.7
$6p_{3/2}$	$9s_{1/2}$	2343.18	7.04[7]	0.4	$4f_{5/2}$	$5g_{7/2}$	4041.25	2.87[9]	0.8	$5d_{5/2}$	$7p_{3/2}$	2796.38	3.10[7]	1.5
$4f_{7/2}$	$6g_{9/2}$	2711.10	1.38[9]	0.2	$5f_{7/2}$	$8d_{5/2}$	5307.19	3.87[7]	0.9	$5s_{1/2}$	$5p_{3/2}$	2817.87	1.17[9]	0.6
$4f_{7/2}$	$6g_{7/2}$	2711.11	3.96[7]	0.2	$5f_{5/2}$	$8d_{3/2}$	5315.96	2.73[7]	1.0	$6p_{1/2}$	$7d_{3/2}$	2868.51	2.19[8]	0.7
$4f_{5/2}$	$6g_{7/2}$	2711.34	1.07[9]	0.2	$5g_{9/2}$	$7f_{7/2}$	5338.62	9.07[6]	3.2	$6p_{3/2}$	$7d_{5/2}$	2914.26	3.69[8]	0.7
$6p_{3/2}$	$7d_{3/2}$	2918.59	4.03[7]	0.7	$5g_{7/2}$	$7f_{5/2}$	5339.15	7.01[6]	3.4	$5s_{1/2}$	$5p_{1/2}$	2946.87	5.10[8]	0.6
$6p_{1/2}$	$8s_{1/2}$	2919.41	6.30[7]	0.3	$6d_{5/2}$	$8p_{3/2}$	5501.70	8.03[6]	1.5	$6f_{7/2}$	$8g_{9/2}$	7604.64	1.88[8]	1.3
$6p_{3/2}$	$8s_{1/2}$	2971.29	1.23[8]	0.3	$6d_{3/2}$	$6f_{5/2}$	5568.81	1.49[8]	2.1	$7d_{5/2}$	$9p_{3/2}$	9443.27	2.70[6]	2.1
$5f_{5/2}$	$8g_{7/2}$	3868.06	2.44[8]	0.3	$4f_{7/2}$	$6d_{5/2}$	5573.80	1.43[8]	0.4					
$5f_{7/2}$	$8g_{9/2}$	3868.06	3.17[8]	0.3	$4f_{5/2}$	$6d_{5/2}$	5574.79	7.14[6]	0.4	$4d_{3/2}$	$8f_{5/2}$	668.73	9.21[8]	1.9
$5f_{7/2}$	$8g_{7/2}$	3868.07	9.05[6]	0.3	$6d_{5/2}$	$6f_{7/2}$	5597.03	2.19[8]	1.7	$4d_{5/2}$	$8f_{7/2}$	671.98	1.33[9]	2.9
$5f_{5/2}$	$7g_{7/2}$	4738.95	3.94[8]	0.7	$6d_{5/2}$	$6f_{5/2}$	5597.61	1.10[7]	1.9	$4d_{3/2}$	$7f_{5/2}$	691.73	1.50[9]	1.6
$5f_{7/2}$	$7g_{9/2}$	4738.95	5.11[8]	0.6	$7d_{3/2}$	$8f_{5/2}$	6523.41	4.68[7]	1.8	$4d_{5/2}$	$7f_{7/2}$	695.20	2.16[9]	2.4
$5f_{7/2}$	$7g_{7/2}$	4738.97	1.46[7]	0.6	$7d_{5/2}$	$8f_{7/2}$	6544.42	6.84[7]	1.4	$4d_{5/2}$	$7f_{5/2}$	695.21	1.06[8]	2.6
$6p_{1/2}$	$6d_{3/2}$	5104.31	6.60[8]	0.8	$7d_{5/2}$	$8f_{5/2}$	6545.13	3.43[6]	1.7	$4d_{3/2}$	$6f_{5/2}$	730.49	2.64[9]	1.2
$6p_{3/2}$	$6d_{5/2}$	5239.56	1.15[9]	0.7	$5f_{7/2}$	$6g_{9/2}$	7256.57	8.65[8]	1.6	$4d_{5/2}$	$6f_{7/2}$	734.37	3.80[9]	1.7
$6p_{3/2}$	$6d_{3/2}$	5265.04	1.27[8]	0.7	$5f_{5/2}$	$6g_{7/2}$	7256.58	6.68[8]	1.6	$4d_{5/2}$	$6f_{5/2}$	734.38	1.88[8]	1.8
$7p_{1/2}$	$8d_{3/2}$	5273.58	8.21[7]	0.5	$5f_{7/2}$	$6g_{7/2}$	7256.63	2.47[7]	1.6	$4d_{3/2}$	$5f_{5/2}$	805.20	5.14[9]	0.6
$7p_{3/2}$	$8d_{5/2}$	5348.56	1.40[8]	0.5	$6f_{5/2}$	$8g_{7/2}$	7603.64	1.45[8]	1.4	$4d_{3/2}$	$7p_{1/2}$	806.18	6.31[7]	2.7
$7p_{3/2}$	$8d_{3/2}$	5357.50	1.53[7]	0.5	$6f_{7/2}$	$8g_{7/2}$	7604.70	5.37[6]	1.3	$4d_{5/2}$	$7p_{3/2}$	808.97	1.31[8]	1.9
$7p_{1/2}$	$9s_{1/2}$	5382.44	2.40[7]	0.3	$5d_{5/2}$	$4f_{5/2}$	7991.61	1.81[7]	0.6	$5p_{3/2}$	$8d_{5/2}$	999.20	2.12[8]	1.5
$6p_{1/2}$	$7s_{1/2}$	5385.14	1.39[8]	0.4	$5d_{5/2}$	$4f_{7/2}$	7993.64	3.63[8]	0.5	$4d_{3/2}$	$6p_{1/2}$	1006.59	1.39[8]	2.4
$7p_{3/2}$	$9s_{1/2}$	5469.89	4.67[7]	0.3	$6g_{9/2}$	$8f_{7/2}$	8647.29	9.41[6]	3.0	$4d_{5/2}$	$6p_{3/2}$	1007.87	2.81[8]	2.1
$6p_{3/2}$	$7s_{1/2}$	5564.36	2.76[8]	0.3	$6g_{7/2}$	$8f_{5/2}$	8648.45	7.27[6]	3.2	$5p_{3/2}$	$7d_{5/2}$	1095.26	4.31[8]	1.2
$6s_{1/2}$	$6p_{3/2}$	7560.80	2.45[8]	0.4	$5g_{9/2}$	$6f_{7/2}$	9041.84	2.08[7]	4.1	$5p_{3/2}$	$7d_{3/2}$	1095.87	4.61[7]	1.3
$6s_{1/2}$	$6p_{1/2}$	7918.89	1.07[8]	0.4	$5g_{7/2}$	$6f_{5/2}$	9043.34	1.61[7]	4.3	$5p_{3/2}$	$6d_{3/2}$	1316.10	1.22[8]	1.0
$5d_{3/2}$	$6p_{3/2}$	8647.45	1.80[7]	0.5	$7d_{3/2}$	$7f_{5/2}$	9653.51	4.31[7]	3.0	$4f_{5/2}$	$8g_{7/2}$	2042.72	3.13[8]	1.0
$5d_{5/2}$	$6p_{3/2}$	8798.62	1.56[8]	0.5	$7d_{5/2}$	$7f_{7/2}$	9699.47	6.39[7]	2.4	$6d_{3/2}$	$8p_{1/2}$	5525.02	3.40[6]	2.0
$5d_{3/2}$	$6p_{1/2}$	9119.09	7.89[7]	0.5	$7d_{5/2}$	$7f_{5/2}$	9701.16	3.21[6]	2.7	$7d_{3/2}$	$9p_{1/2}$	9492.86	1.07[6]	2.4
$7p_{1/2}$	$7d_{3/2}$	9837.57	2.05[8]	0.7	$5f_{5/2}$	$7d_{5/2}$	9935.59	4.37[6]	0.9					
					$5f_{7/2}$	$7d_{5/2}$	9935.69	8.74[7]	0.7					
					$5f_{5/2}$	$7d_{3/2}$	9986.07	6.18[7]	0.9					

are calculated using

$$gA_r = \frac{2.02613 \times 10^{18}}{\lambda^3} \times S \ \mathrm{s}^{-1}, \qquad (1)$$

where the wavelength λ is in Å and the line strength $S = D^2$ is in atomic units.

Transition rates gA (s^{-1}) for the 141 allowed electric-dipole transitions between ns, np_j, nd_j, nf_j, and ng_j

TABLE IV: Weighted oscillator strengths gf in Y III calculated using our recommended values of reduced electric-dipole matrix elements are compared with "HFR+Pol" results [9] and the WBEPM semi-empirical results [10]. Uncertainties are given in parenthesis.

Transition		Oscillator Strengths		
Lower	Upper	Final	RHF+Pol [9]	WBEPM [10]
$4d_{3/2}$	$4f_{5/2}$	1.553(6)	1.5389	
$4d_{5/2}$	$4f_{5/2}$	0.1131(5)	0.1091	
$4d_{5/2}$	$4f_{7/2}$	2.266(11)	2.1834	
$4d_{3/2}$	$6p_{1/2}$	0.0211(5)	0.0311	
$4d_{5/2}$	$6p_{3/2}$	0.0428(9)	0.0560	
$5p_{1/2}$	$5d_{3/2}$	2.096(13)	2.2533	1.8186
$5p_{3/2}$	$5d_{5/2}$	3.835(23)	3.9390	3.3504
$5p_{3/2}$	$5d_{3/2}$	0.428(2)	0.4358	0.3745
$5p_{1/2}$	$6s_{1/2}$	0.391(3)	0.4390	0.3074
$5p_{3/2}$	$6s_{1/2}$	0.832(5)	0.8478	0.6636
$4d_{3/2}$	$5p_{3/2}$	0.0959(7)	0.1054	
$4d_{5/2}$	$5p_{3/2}$	0.871(7)	0.9322	
$4d_{3/2}$	$5p_{1/2}$	0.476(3)	0.5077	
$5s_{1/2}$	$5p_{3/2}$	1.390(8)	1.4761	1.5012
$5s_{1/2}$	$5p_{1/2}$	0.664(4)	0.7056	0.7202
$6s_{1/2}$	$6p_{3/2}$	2.098(9)	2.1914	
$6s_{1/2}$	$6p_{1/2}$	1.008(4)	1.0464	
$5d_{3/2}$	$4f_{5/2}$	2.466(13)	2.6970	2.5388
$5d_{5/2}$	$4f_{5/2}$	0.174(1)	0.1897	0.1788
$5d_{5/2}$	$4f_{7/2}$	3.473(19)	3.7964	3.9642
$5d_{3/2}$	$6p_{3/2}$	0.201(10)	0.2196	
$5d_{5/2}$	$6p_{3/2}$	1.807(9)	1.9429	
$5d_{3/2}$	$6p_{1/2}$	0.984(5)	1.0414	

states with $n \leq 8$ are listed in Table III. Vacuum wavelengths obtained from NIST energies are also listed for reference. The transitions are ordered by the value of the wavelength. The relative uncertainties of the transition rates are twice of the corresponding matrix element uncertainties. The uncertainties in per cent are listed in the column labeled "Unc.". The largest uncertainties (about 2%) are for the $4d_j - nf_{j'}$ transitions, while the smallest ones (about 0.3%) are for the $5p_j - ns$ transitions as we discussed in the previous section. The larger uncertainties generally results from the larger relative size of the correlation corrections.

The 141 allowed electric-dipole transitions between ns, np_j, nd_j, nf_j, and ng_j states displayed in Table III are compared with gA_r values presented in Table 6 of Ref. [9].

Those theoretical transition probabilities in Y III were obtained using a multiconfiguration relativistic Hartree-Fock method including core polarization. We did not repeat gA_r[9] values from Table 6 of Ref. [9], however, we presented our $gA_r^{\rm final}$ values accordingly the level of the disagreement with results from [9]. In the left column of Table III, we displayed $gA_r^{\rm final}$ values for 47 transitions. The correlation corrections for these transitions contribute less than 10%. As a result, the difference between our $gA_r^{\rm final}$ values and the gA_r values from [9] is also less than 10%. In the second column of Table III, we present 49 transitions. We find substantially larger disagreement (11%-40%) between $gA_r^{\rm final}$ and gA_r[9]. However, the gA_r values from [9] are in the good agreement with $gA_r^{\rm DF}$ values. To make this determination, we used the reduced matrix elements obtained in the DF approach given in Table II to calculated $gA_r^{\rm DF}$ values using DF values for matrix elements and NIST energies. We find small (less than 10%) differences for the 49 transitions displayed in the second column of Table III between the gA_r[9] and $gA_r^{\rm DF}$ values. Therefore, these differences is attributed to omitted higher-order correlation corrections in [9]. The best agreement (less than 10%) between $gA_r^{\rm final}$ and gA_r[9] is found for the 25 transitions displayed in the top of third column of Table III, while the contribution of correlation effects (the $gA_r^{\rm final}$ and $gA_r^{\rm DF}$difference) are 11% - 40%. The gA_r[9] values are in disagreements with $gA_r^{\rm final}$ and $gA_r^{\rm DF}$ values for the 20 transitions displayed in the bottom of third column of Table III. The correlation corrections are particulary large for these cases, leading to large uncertainties shown in column "Unc." of Table III.

In Table IV, we present weighted oscillator strengths gf for transitions in Y III calculated using our recommended values of reduced electric-dipole matrix elements $f^{\rm final}$ and their uncertainties which are given in parenthesis. We compare our results with the theoretical oscillator strengths obtained using a multiconfiguration relativistic Hartree-Fock method including core polarization [9] ("RHF+Pol." column) and WBEPM method [10]. The WBEPM is a non-relativistic semi-empirical method that uses parameters obtained by fitting of the experimental energy data. Only few oscillator strengths values are listed in [10]. We find large discrepancies (about 15%-40%) between WBEPM results and all other results given in Table IV for the $5p - 5d$ and $5p - 6s$ transitions, while the "Final"and "RHF+Pol." agreement is good (1%-7%) for these transitions. Oscillator strengths for the $5s - 5p$ and $5d - 4f$ transitions agree which each other to 2%-12%.

C. Lifetimes in Rb-like Y III

We calculated lifetimes of the ns ($n = 6 - 9$), np_j ($n = 5 - 9$), nd_j ($n = 5 - 8$), nf_j ($n = 4 - 8$), and ng_j ($n = 5 - 8$) states in Y III using out final values of the transition rates listed in Table III. The lifetimes of the metastable $4d_{5/2}$ and $5s$ states are discussed in the next section. The uncertainties in the lifetime values are obtained from the uncertainties in the transition rates listed in Table III. We also included the lowest-order DF lifetimes $\tau^{\rm DF}$ to illustrate the size of the correlation effects. The recommended NIST energies [8] are given in column 'Energy' for reference. Our final results are given in columns $\tau^{\rm final}$ Table V.

The present values are compared with theoretical results obtained by Biémont *et al.* [9] using the multiconfiguration relativistic Hartree-Fock method including core polarization (see column $\tau^{\rm theory}$ in Table V). We

TABLE V: Lifetimes ($\tau^{\rm final}$ in nsec) of nl_j states in Rb-like Y III. Uncertainties are given in parenthesis. Recommended NIST energies [8] are given in cm^{-1}. The values of lifetimes evaluated in the DF approximation are given in column $\tau^{\rm DF}$ to illustrate the importance of the correlation corrections. Theoretical values from Ref. [9] and experimental measurements from Refs. [9, 11] are listed in the two last columns.

Level	Energy [8]	$\tau^{\rm DF}$	$\tau^{\rm final}$	$\tau^{\rm theory}$[9]	$\tau^{\rm expt}$
$5p_{1/2}$	41401.46	1.449	1.898(9)	1.78	1.9(1)[9]
$5p_{3/2}$	42954.87	1.324	1.723(8)	1.61	1.8(2)[9]
$6s_{1/2}$	86717.59	1.224	1.253(6)	1.19	1.23(8)[11]
$5d_{3/2}$	88379.61	0.962	1.089(6)	1.02	0.93(7)[11]
$5d_{5/2}$	88578.29	1.000	1.127(7)	1.10	1.06(8)[11]
$6p_{1/2}$	99345.62	4.488	5.565(55)	4.80	
$6p_{3/2}$	99943.71	4.136	5.229(42)	4.51	
$4f_{5/2}$	101088.23	0.387	0.517(2)	0.53	
$4f_{7/2}$	101091.42	0.387	0.514(3)	0.52	
$7s_{1/2}$	117915.23	1.862	1.856(3)	1.79	
$6d_{3/2}$	118936.91	1.985	2.361(11)	2.22	
$6d_{5/2}$	119029.30	2.072	2.469(13)	2.33	
$7p_{1/2}$	124041.76	9.229	11.05(11)	9.50	
$5f_{5/2}$	124192.92	0.638	0.940(4)	0.88	
$5f_{7/2}$	124193.02	0.640	0.934(7)	0.89	
$7p_{3/2}$	124338.78	8.680	10.75(9)	9.15	
$5g_{7/2}$	125836.22	2.300	2.684(20)	1.37	
$5g_{9/2}$	125836.15	2.303	2.686(19)	2.37	
$8s_{1/2}$	133599.09	2.947	2.906(4)	2.82	
$7d_{3/2}$	134206.87	3.555	4.362(18)	4.07	
$7d_{5/2}$	134257.75	3.740	4.586(22)	4.23	
$6f_{5/2}$	136894.08	1.023	1.621(14)	1.42	
$6f_{7/2}$	136895.91	1.026	1.606(21)	1.44	
$8p_{1/2}$	137036.4	16.18	18.90(20)	16.32	
$8p_{3/2}$	137205.5	15.47	18.91(19)	15.94	
$6g_{7/2}$	137973.52	3.933	4.449(27)	4.10	
$6g_{9/2}$	137973.63	3.934	4.450(27)	4.10	
$9s_{1/2}$	142620.7	4.502	4.417(5)	4.30	
$8d_{3/2}$	143004.2	5.782	7.224(31)	6.70	
$8d_{5/2}$	143035.4	6.082	7.597(40)	6.91	
$7f_{5/2}$	144565.80	1.560	2.607(28)	2.19	
$7f_{7/2}$	144567.59	1.566	2.577(43)	2.22	
$9p_{1/2}$	144741.1	25.76	29.72(36)	25.75	
$9p_{3/2}$	144847.3	24.94	29.85(16)	25.36	
$7g_{7/2}$	145294.65	6.204	6.827(39)	6.49	
$7g_{9/2}$	145294.73	6.211	6.831(40)	6.49	
$8f_{5/2}$	149536.28	2.280	3.937(46)	3.17	
$8f_{7/2}$	149537.94	2.286	3.905(73)	3.20	
$8g_{7/2}$	150045.68	9.211	9.962(57)	9.66	
$8g_{9/2}$	150045.78	9.217	9.957(54)	9.66	

find good agreement (2%-8%) between $\tau^{\rm final}$ and lifetimes from [9] for the ns ($n = 6-9$), $5p_j$, nd_j ($n = 5-8$), nf_j ($n = 4-5$), and ng_j $n = 6-8$) states. Lifetimes of the $6p$, $7p$, $8p$, and $9p$ states presented by Biémont *et al.* [9] disagree substantially (13%-15%) with our results, however they are in very good agreement (0% -9%) with the $\tau^{\rm DF}$. This may indicate that some dominant correlation corrections were missing in [9] for these states. We noticed the misprint for the lifetime of the $5g_{7/2}$ level in [9] (it should be 2.37 instead of 1.37).

There are only few experimental measurements for lifetimes of Rb-like Y III presented recently by Biémont *et al.* [9] and by Maniak *et al.* [11]. Our $\tau^{\rm final}$ values are in the perfect agreement with these measurements when uncertainties are taken into account.

IV. ELECTRIC-QUADRUPOLE AND MAGNETIC-DIPOLE MATRIX ELEMENTS

The M1 $4d_{3/2} - 4d_{5/2}$, $4d_{3/2} - 5s$ and E2 $4d_{3/2} - 4d_{5/2}$, $4d_j - 5s$ matrix elements are evaluated using the same approach as for the E1 matrix elements. In Table VI, we list results for the magnetic-dipole (M1) and electric-quadrupole (E2) matrix elements calculated in different approximations: lowest-order DF, second-order RMBPT, third-order RMBPT, and all-order method with and without the triple excitations. The scaled all-order values are indicated by the label "sc". Final recommended values and their uncertainties are given in the $Z^{\rm final}$ column. The last column gives relative uncertainties of the final values in %. The final value of the M1 $4d_{3/2} - 4d_{5/2}$ matrix element is the same as the lowest order DF result. The M1 matrix element for the $4d_{3/2}-4d_{5/2}$ transition changes substantially with the inclusion of the correlations. The value of the M1 $4d_{3/2}-5s$ matrix element is not zero due to relativistic effects; it is smaller than the value of the M1 $4d_{3/2} - 4d_{5/2}$ matrix element by five orders of magnitude. Our procedure for estimating the uncertainty described in Ref. [32] can not be applied to this matrix element since different correlation corrections dominate for this transition. However, the contribution of this transition to the $5s$ lifetime is negligible. For all three E2 transitions considered here, a single correlation correction term that can be improved by the scaling strongly dominates. Therefore, we can use uncertainty estimate procedure described in [32]. The present values are compared with CCSDpT calculations of Ref. [12]. Our values for the electric-quadrupole matrix elements are in agreement with the results of Ref. [12].

We combine recommended NIST energies [8] and our final values of the matrix elements listed in Table VI to calculate transition rates A given by

$$A(M1) = \frac{2.69735 \times 10^{13}}{(2J+1)\lambda^3}\, S(M1), \qquad (2)$$

$$A(E2) = \frac{1.11995 \times 10^{18}}{(2J+1)\lambda^5} S(E2), \qquad (3)$$

where the wavelength λ is in Å and the line strength $S = Z^2$ is in atomic units. Transition rates A (in s^{-1}) for the M1 $4d_{3/2} - 4d_{5/2}$ and $4d_{3/2} - 5s_{1/2}$ transitions and the E2 $4d_{3/2} - 4d_{5/2}$, $4d_{3/2} - 5s_{1/2}$ and $4d_{5/2} - 5s_{1/2}$ transitions in Y III are summarized in Table VII. Final lifetimes of the $4d_{5/2}$ and $5s$ levels are also given (in s). Uncertainties are given in parenthesis.

TABLE VI: E2 and M1 reduced matrix elements in Rb-like Y III in atomic units calculated in different approximations. Absolute values are given. The lowest-order DF, second-order, third-order MBPT, and all-order SD and SDpT values are listed; the label "sc" indicates the scaled values. Final recommended values and their uncertainties are given in the $Z^{\rm final}$ column. The last column gives relative uncertainties of the final values in %.

Transition		$Z^{\rm DF}$	$Z^{\rm (DF+2)}$	$Z^{\rm (DF+2+3)}$	$Z^{\rm SD}$	$Z^{\rm (SD)}_{\rm sc}$	$Z^{\rm SDpT}$	$Z^{\rm SDpT}_{\rm sc}$	$Z^{\rm final}$	Unc. (%)
Magnetic-dipole transitions										
$4d_{3/2}$	$4d_{5/2}$	1.5490	1.5490	1.5373	1.5491	1.5491	1.5491	1.5491	1.5491(0)	0
$4d_{3/2}$	$5s_{1/2}$	6.147[-6]	3.327[-5]	7.925[-3]	3.964[-5]	3.948[-5]	3.940[-5]	3.956[-5]	3.95[-5]	
Electric-quadrupole transitions										
$4d_{3/2}$	$4d_{5/2}$	3.5310	3.4205	3.0522	3.1059	3.1145	3.1234	3.1075	3.114(9)	0.29
$4d_{3/2}$	$5s_{1/2}$	6.6882	6.0368	5.9282	6.0537	6.0761	6.0948	6.0637	6.08(2)	0.31
$4d_{5/2}$	$5s_{1/2}$	8.2696	7.5032	7.3464	7.4978	7.5231	7.5477	7.5078	7.52(2)	0.33

TABLE VII: M1 and E2 transition rates A (in s^{-1}) and $5s$ and $4d_{5/2}$ lifetimes τ (in s) in Rb-like Y III. Uncertainties are given in parenthesis. Our values are compared with theoretical results from Ref. [12]

	Transition		Present	Ref. [12]
A(E2)	$4d_{3/2}$	$4d_{5/2}$	3.61(2)[-8]	3.7011[-8]
A(M1)	$4d_{3/2}$	$4d_{5/2}$	4.0963[-3]	4.0667[-3]
Lifetime (in s)	$4d_{5/2}$		244.1	245.89
A(M1)	$4d_{3/2}$	$5s_{1/2}$	8.75(4)[-8]	6.2522[-7]
A(E2)	$4d_{3/2}$	$5s_{1/2}$	4.80(3)[-2]	4.8952[-2]
A(E2)	$4d_{5/2}$	$5s_{1/2}$	4.42(3)[-2]	4.5090[-2]
Lifetime (in s)	$5s_{1/2}$		10.85(7)	10.63

Our transition rate and lifetime values are compared with CCSDpT results presented by Sahoo *et al.* [12]. The only substantial difference between our final result and the CCSDpT result is for the M1 $4d_{3/2} - 5s_{1/2}$ transition rate. For this transition, correlation correction is actually larger than the DF value. Therefore, this value is extremely sensitive to the treatment of the correlation correction which differs between our approach and that of Ref. [12], as large differences of the results are expected. The contribution of the M1 $4d_{3/2} - 5s_{1/2}$ transition to the $5s$ lifetime is negligible and this difference does not not affect the lifetime value. Our values of the $5s$ and $4d_{5/2}$ lifetimes are in agreement with Ref. [12] results.

V. STATIC MULTIPOLE POLARIZABILITIES OF THE $5s$ STATE

The static multipole polarizability α^{Ek} of Rb-like Y III in its $5s$ state can be separated into two terms; a dominant first term from intermediate valence-excited states, and a smaller second term from intermediate core-excited states. The core term is smaller than the former one by several orders of magnitude and is evaluated here in the random-phase approximation [33]. The dominant valence contribution is calculated using the sum-over-state approach

$$\alpha^{Ek}_v = \frac{1}{2k+1} \sum_n \frac{|\langle nl_j \| r^k C_{kq} \| 5s \rangle|^2}{E_{nlj} - E_{5s}}, \qquad (4)$$

where $C_{kq}(\hat{r})$ is a normalized spherical harmonic and where nl_j is np_j, nd_j, and nf_j for $k = 1$, 2, and 3, respectively [34]. The reduced matrix elements in the dominant contributions to the above sum are evaluated using out final values of the matrix elements and NIST energies

TABLE VIII: Contributions to multipole polarizabilities of the $5s$ state of Rb-like Y III in a_0^3. Uncertainties are given in parenthesis.

Contr.	α^{E1}
$5p_{1/2}$	13.90(8)
$5p_{3/2}$	26.59(15)
$(6-26)p_j$	0.15(0)
Tail	0.00
Term-vc	-0.17
Core	4.05
Total	44.5(2)
Contr.	**α^{E2}**
$4d_{3/2}$	-217.0(1.3)
$5d_{3/2}$	62.3(1)
$(6-26)d_{3/2}$	4.1(0)
$4d_{5/2}$	-368.4(2.4)
$5d_{5/2}$	92.3(1)
$(6-26)d_{5/2}$	6.3(0)
Tail	-0.01
Core	9.5
Total	430(3)
Contr.	**α^{E3}**
$4f_{5/2}$	1304(8)
$5f_{5/2}$	9(1)
$(6-26)f_{5/2}$	32(0)
$4f_{7/2}$	1739(10)
$5f_{7/2}$	12(1)
$(6-26)f_{7/2}$	42(0)
Tail	2
Core	50
Total	3191(13)

TABLE IX: Contributions to the $4d_j$ scalar and tensor polarizabilities of Rb-like Y III in a_0^3. $np_j = (7-26)p_j$ and $nf_j = (7-26)f_j$. Uncertainties are given in parenthesis.

Contr.	α_0	Contr.	α_2	Contr.	α_0	Contr.	α_2
	$4d_{3/2}$		$4d_{3/2}$		$4d_{5/2}$		$4d_{5/2}$
$5p_{1/2}$	3.343(24)	$5p_{1/2}$	-3.343(24)	$5p_{3/2}$	3.920(31)	$5p_{3/2}$	-3.920(31)
$6p_{1/2}$	0.026(1)	$6p_{1/2}$	-0.026(1)	$6p_{3/2}$	0.035(1)	$6p_{3/2}$	-0.035(1)
$np_{1/2}$	0.062(0)	$np_{1/2}$	-0.062(0)	$np_{3/2}$	0.056(0)	$np_{3/2}$	-0.056(0)
$5p_{3/2}$	0.626(5)	$5p_{3/2}$	0.505(4)	$4f_{5/2}$	0.090(0)	$4f_{5/2}$	0.103(0)
$6p_{3/2}$	0.006(0)	$6p_{3/2}$	0.005(0)	$5f_{5/2}$	0.019(0)	$5f_{5/2}$	0.022(0)
$np_{3/2}$	0.011(0)	$np_{3/2}$	0.010(0)	$6f_{5/2}$	0.007(0)	$6f_{5/2}$	0.008(0)
				$nf_{5/2}$	0.015(0)	$nf_{5/2}$	0.018(0)
$4f_{5/2}$	1.830(7)	$4f_{5/2}$	-0.366(1)	$4f_{7/2}$	1.806(9)	$4f_{7/2}$	-0.645(3)
$5f_{5/2}$	0.390(2)	$5f_{5/2}$	-0.078(0)	$5f_{7/2}$	0.382(3)	$5f_{7/2}$	-0.136(1)
$6f_{5/2}$	0.136(2)	$6f_{5/2}$	-0.027(0)	$6f_{7/2}$	0.133(2)	$6f_{7/2}$	-0.047(1)
$nf_{5/2}$	0.306(0)	$nf_{5/2}$	-0.061(0)	$nf_{7/2}$	0.346(0)	$nf_{7/2}$	-0.124(0)
Main	6.734(26)	Main	-3.448(24)	Main	6.809(32)	Main	-4.813(31)
Core	4.048	Core	0	Core	4.048	Core	0
α_{vc}	-0.313	α_{vc}	0	α_{vc}	-0.341	α_{vc}	0
Tail	0.008	Tail	-0.002	Tail	0.006	Tail	-0.002
Total	10.48(3)	Total	-3.45(2)	Total	10.52(3)	Total	-4.81(3)

[8]. The uncertainties in the polarizability contributions are obtained from the uncertainties in the corresponding matrix elements. The final values for the quadrupole and octupole matrix elements and their uncertainties are determined using the same procedure as for the dipole matrix elements.

Contributions to dipole, quadrupole, and octupole polarizabilities of the $5s$ ground state are presented in Table VIII. The first two terms in the sum-over-states for α^{E1}, and α^{E3} contribute 99.6% and 96.95%, respectively, of the totals. The remaining 3.1% of α^{E3} contribution comes from the (5-26)nf_j states. In the case of α^{E2}, the contribution of the $4d_j$ and $5d_j$ states slightly cancel each other. The remaining 2.5% of α^{E2} contributions are from the (6-26)nd_j states. We use recommended energies from [8] and our final matrix elements to evaluate terms in the sum with $n \leq 13$, and we use theoretical SD energies and matrix elements to evaluate terms with $13 \leq n \leq 26$. The remaining contributions to α^{Ek} from orbitals with $27 \leq n \leq 70$ are evaluated in the RPA approximation since the contributions from these terms are smaller than 0.01% in all cases. These terms are grouped together as "Tail". We evaluate core contributions in the random-phase approximation [33] for E1, E2, and E3. Our result for core E1 polarizability is the same as in [33]. The core polarizabilities are small in comparison with the valence ones and their uncertainties are negligible. We note that α_{vc} terms are zero for the E2 and E3 polarizabilities since Rb-like Y III core contains no nd or nf states.

VI. SCALAR AND TENSOR EXCITED STATE POLARIZABILITIES

The valence scalar $\alpha_0(v)$ and tensor α_2 polarizabilities of an excited state v of Rb-like Y III are given by

$$\alpha_0(v) = \frac{2}{3(2j_v+1)} \sum_{nlj} \frac{|\langle v||rC_1||nlj\rangle|^2}{E_{nlj} - E_v} \qquad (5)$$

$$\alpha_2 = (-1)^{j_v} \sqrt{\frac{40 j_v (2j_v-1)}{3(j_v+1)(2j_v+1)(2j_v+3)}} \times \sum_{nlj} (-1)^j \left\{ \begin{array}{ccc} j_v & 1 & j \\ 1 & j_v & 2 \end{array} \right\} \frac{|\langle v||rC_1||nlj\rangle|^2}{E_{nlj} - E_v} \,. \qquad (6)$$

The excited state polarizability calculations are carried out in the same way as the calculations of the multipole polarizabilities discussed in the previous section. We list the contributions to the $4d_j$ scalar and tensor polarizabilities of Rb-like Y III in Table IX. The dominant contributions are listed separately. The first three terms ($5p_{1/2}$, $5p_{3/2}$, and $4f_{5/2}$) in the sum-over-states for $\alpha_0(4d_{3/2})$ and $\alpha_2(4d_{3/2})$ contribute 86% and 93%, respectively, of the totals. The other four ($6p_{1/2}$, $6p_{3/2}$, $5f_{5/2}$ and $6f_{5/2}$) terms displayed in Table IX for $\alpha_0(4d_{3/2})$ and $\alpha_2(4d_{3/2})$ contribute 8.3% and 3.7%, respectively, of the totals. The remaining contributions are grouped together. For example, "$np_{1/2}$" contribution includes all of the $np_{1/2}$ terms excluding only the terms that were already listed separately. These remaining contributions ($np_{1/2}$, $np_{3/2}$, and $nf_{5/2}$ with n = 7-26) are equal to 5.6% and 3.3%, respectively, of the totals. We evaluate contribution from

ionic core $\alpha_{\rm core}$ in the RPA and find $\alpha_{\rm core} = 4.05\ a_0^3$. The "Tail" contribution (n = 27-65) is very small (less than 0.1%). The largest contribution of the $\alpha_{\rm vc}$ term is for the $4d$ states [$\alpha_{vc}(4d_{3/2})$ = -0.31 a_0^3].

VII. CONCLUSION

In summary, we carried out a systematic high-precision relativistic study of Rb-like Y III atomic properties for the ns, np_j, nd_j, nf_j, and ng_j ($n \leq$8) states using an all-order approach and evaluated uncertainties of our recommended values. The theoretical energy values are in excellent agreement with existing experimental data. Reduced matrix elements, oscillator strengths, transition rates, and lifetimes for the first low-lying levels up to n =8 are calculated. Electric-dipole ($5s - np_j$, $n = 5-26$), electric- quadrupole ($5s - nd_j$, $n = 4-26$), and electric-octupole ($5s - nf_j$, $n = 4-26$) matrix elements are calculated to obtain the ground state E1, E2, and E3 static polarizabilities. Scalar and tensor polarizabilities of the $4d_{3/2}$ and $4d_{5/2}$ states of Rb-like Y III are evaluated. Particular care was taken to accurately treat contributions from highly-excited states. The uncertainties are evaluated for most of the values listed in this work. This work provides recommended values for a number of atomic properties via a systematic high-precision study for use in planning and analysis of various experiments as well as theoretical modeling.

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